1,4-Dioxane
123-91-1 | DTXSID4020533

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 42.0 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.36e-01

Confidence level: 8.10e-01

Nearest Neighbors from the Training Set

Image not found
Butyl acetate
Measured: 38.1
Predicted: 16.4

Image not found
2-Ethyl-2-hexenal
Measured: 79.0
Predicted: 1.35

Image not found
Fluorobenzene
Measured: 34.1
Predicted: 58.3

Image not found
2-Butyne-1,4-diol
Measured: 48.0
Predicted: 2.85e-03

Image not found
Ethyl butyrate
Measured: 27.6
Predicted: 14.7